Solving Langevin equation with the bicolour rooted tree method

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Abstract

Stochastic differential equations, especially the one called Langevin equation, play an important role in many fields of modern science. In this paper, we use the bicolour rooted tree method, which is based on the stochastic Taylor expansion, to get the systematic pattern of the high order algorithm for Langevin equation. We propose a popular test problem, which is related to the energy relaxation in the double well, to test the validity of our algorithm and compare our algorithm with other usually used algorithms in simulations. And we also consider the time-dependent Langevin equation with the Ornstein-Uhlenbeck noise as our second example to demonstrate the versatility of our method.

1. Introduction

Nature is full of randomness, from nucleus to whole galaxy, from inorganism to organism and from the domain of science and technology to the human society [1, 2, 3, 4, 5, 6, 7, 8]. Although the mechanisms of randomness are different from one field to another, the ways to describe them are similar. The stochastic differential equation (SDE) is a good approach to describe the randomness. The earliest work on SDEs was done to describe Brownian motion in Einstein's famous paper and at the same time by Smoluchowski.

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Later Itô and Stratonovich put SDEs on a more solid theoretical foundation. In 1908, a French physicist, Paul Langevin, developed an equation called the Langevin equation (LE) thereafter, which incorporated a random force into the Newton equation, to describe the Brownian motion. Langevin equation is an equation to mechanics using simplified models and using SDEs to account for omitted degrees of freedom. There are many branches with rich contents which have been derived in the last 100 years. For example, the reaction kinetic dynamics in chemistry [9], the molecular motor and protein folding in biology [10, 11], the intracellular and intercellular calcium signaling, quantum Brownian motion and the stochastic quantization in physics [12, 13, 14], even the stock market fluctuations and crashes [8] are all related to the Langevin equation. The Langevin equation plays an important role in modern science, however only a few of them can be analytically solved, thus it is necessary to develop a numerical algorithm which incorporates both the computation efficiency and accuracy.

The general structure of the stochastic differential equation is

$$\dot{x}_i = f_i(X(t)) + g_i(X(t))\xi_i(t) \quad (i = 1, 2, ..., d), \tag{1}$$

where $X(t) = \{x_1, x_2, ..., x_d\}$, $f_i(X(t))$s are the deterministic part of the equations of motion, $g_i(X(t))$s are the diffusion coefficients and $\xi_i(t)$s are a set of independent gaussian random variables with correlation function

$$< \xi_i(t)\xi_j(t^{'}) > = \delta_{ij}\delta(t - t^{'}). \tag{2}$$

To get a certain order algorithm for the SDE, we can directly do the stochastic Taylor expansion of Eq.(1) to our desired accuracy [15, 16]. This method is very explicit and suits for many cases of the SDEs, however, since this expansion is too laborious to generate to high orders, we need to find a systematic pattern to overcome such difficulty. In this paper, we use the bicolour rooted tree method (BRT) based on the stochastic Taylor expansion to obtain the high order algorithm for SDEs systematically.

In the field of numerical method for solving ordinary differential equations, J. C. Butcher develops a rooted tree method which relates each term in the ordinary Taylor expansion to a rooted tree [17]. His method can excellently make the laborious ordinary Taylor expansion systematic in a heuristic way. Then K. Burrage and P. M. Burrage expand the rooted-tree method to the bicolour rooted tree method which relates each term in the stochastic Taylor expansion to a bicolour rooted tree [16] for the sake of solving SDE.

They give an explicit Runge-Kutta method of order 2.5 in their paper for the SDE. In this paper, we further develop their works, propose a new type of the bicolour rooted tree method, and apply it to the LE case.

Since the intricacy of the numerical method for SDE, the order of it is heretofore not great than 2.5 [16, 18]. But for some special kinds of the SDE, for example, the Langevin equation, a high order algorithm can be acquired. Hershkovitz has developed a fourth order algorithm for the LE [15], which is based on the stochastic Taylor expansion. In this paper, we use the BRT method to improve the accuracy to order 7 of deterministic part and order 4.5 of stochastic part ($o(7,4.5)$).

In section 2, we briefly introduce the BRT method and explore the relation between the terms in the stochastic Taylor expansion and the bicolour rooted trees. We find that the stochastic Taylor expansion is just equal to the sum of all the non-isomorphic bicolour rooted trees. In section 3, due to the structure of LE, we can use the BRT method to obtain our algorithm $o(7,4.5)$ for the LE. In section 4, we use two examples to verify the validity and demonstrate the versatility of our algorithm. The first one is the energy relaxation in the double well. We compare our results with the previous results obtained by other algorithms and show the convergence of these different algorithms. The second one we present an algorithm for the time-dependent Langevin equation with the Ornstein-Uhlenbeck noise, and our results are readily agreed with the previous ones.

2. Bicolour rooted tree method

To cope with the intricacy of the Taylor expansion of SDE, a method which is called bicolour rooted tree method (BRT) [16] based on the rooted tree method [17] developed by J. C. Butcher is introduced to conveniently do the stochastic Taylor expansion of SDE.

Let us firstly transform the Eq.(1) into the following equation,

$$dx_i = f_i(X(t))dt + g_i(X(t)) \circ dW_i(t) \quad (i = 1, 2, ..., d), \qquad (3)$$

where $W_i(t)$ is the Wiener process, and the symbol $\circ$ implies that the SDE considered in this paper is in the Stratonovich sense, for the Stratonovich integral satisfies the usual rules of calculus [18]. One can therefore integrate Eq.(3) from 0 to h,

$$x_i(h) - x_i(0) = \int_0^h f_i(X(s))ds + \int_0^h g_i(X(s)) \circ dW_i(s). \qquad (4)$$

Taylor expansion of the functions gives,

$$f_i(X(s)) = \sum_{n=0}^{\infty} \frac{1}{n!} (\sum_{m=1}^{d} \delta x_m \frac{\partial}{\partial x_m})^n f_i(X(0)), \tag{5}$$

$$g_i(X(s)) = \sum_{n=0}^{\infty} \frac{1}{n!} (\sum_{m=1}^{d} \delta x_m \frac{\partial}{\partial x_m})^n g_i(X(0)). \tag{6}$$

Now taking the last two equations into Eq.(4), one can easily get

$$\delta x_i(h) = x_i(h) - x_i(0) =$$
$$\int_0^h (f^i + f_j^i \delta x_j(s) + \frac{1}{2!} f_{jk}^i \delta x_j(s) \delta x_k(s) + \cdots) ds + \tag{7}$$
$$\int_0^h (g^i + g_j^i \delta x_j(s) + \frac{1}{2!} g_{jk}^i \delta x_j(s) \delta x_k(s) + \cdots) \circ dW_i(s),$$

where $f^i \equiv f_i(X(0)), f_{jk}^i \equiv \frac{\partial}{\partial x_j} \frac{\partial}{\partial x_k} f_i(X(0))$ and the repeated indices except i (the number of the equations) imply the Einstein's summation convention throughout the paper.

Then the terms with 0th derivative in Eq.(7) are,

$$\delta x_i^0(h) = f^i J_{0,h} + g^i J_{i,h}, \tag{8}$$

where $J_{0,h} = \int_0^h ds$ and $J_{i,h} = \int_0^h \circ dW_i(s)$, so $\delta x_i(h) = \delta x_i^0(h) + \cdots$, substituting it for Eq.(7) gives the 1st derivative terms,

$$\delta x_i^1(h) = f_j^i f^j J_{00,h} + f_j^i g^j J_{j0,h} + g_j^i f^j J_{0i,h} + g_j^i g^j J_{ji,h}, \tag{9}$$

where $J_{j_1 j_2 \cdots j_k, t}$ is the Stratonovich multiple integral [18], and the integration is with respect to ds if $j_l = 0$ or $\circ dW_i(s)$ if $j_l = i$, for example,

$$J_{012,t} = \int_0^t \circ dW_2(s_1) \int_0^{s_1} \circ dW_1(s_2) \int_0^{s_2} ds_3. \tag{10}$$

Replacing Eq.(7) by $\delta x_i(h) = \delta x_i^0(h) + \delta x_i^1(h) + \cdots$, one can get the 2nd derivative terms $\delta x_i^2(h)$ and performing this procedure recursively will generate all the derivative terms in principle. However, close calculation of these derivative terms reveals that the complexity will increase drastically as the order rises. For this reason, we adopt the BRT method developed by J. C.

4

Butcher and P. M. Burrage to express each derivative term systematically and graphically.

We will first introduce some useful notations [16]. Take the bicolour rooted tree t in Fig.1 as an example, The tree has 8 vertices, each vertex can be colored by white node ($\circ$) or black node ($\bullet$) which is the representative of stochastic node (σ) or deterministic node (τ). If $t_1, \cdots, t_m$ are bicolour rooted trees, then $[t_1, \cdots, t_m]$ and $\{t_1, \cdots, t_m\}$ are trees in which $t_1, \cdots, t_m$ are each joined by a single branch to $\bullet$ or $\circ$, respectively. We can therefore rewrite the tree t in a compact form $[\sigma, [\{\sigma\}, [\tau, \sigma]]]$. To conveniently calculate the weight of this tree, we define the following terms: the *degree* of the vertex $C(v)(v \in t)$ in the BRT is equivalent to the degree of vertex $D(v)$ in the graph theory except the root 1 with $C(1) = 1 + D(1)$. S is the *symmetry factor* of the tree t, for example, the trees interchanged the branches joint to vertex 1 or 3 or 5 are regarded as identical with tree t, therefore the symmetry factor of tree t is $2 \times 2 \times 2 = 8$. Then tracing the stochastic Taylor expansion of the Eq.(7), we find that the *elementary weight* of the tree, which is also the coefficient of each term in the expansion, is

$$a(t) = S \prod_{i=1}^{n} \frac{1}{(C(v_i) - 1)!}, \tag{11}$$

where n is the total number of vertex in the tree and vertex $v_i \in t$. Now we introduce the *elementary derivative* and *elementary integral* here [16]. An elementary derivative $F(t)$ can be associated with a BRT such that

$$F(\tau) = f, F(\sigma) = g,$$
$$F(t) = \begin{cases} f^{(m)}[F(t_1), \cdots, F(t_m)], t = [t_1, \cdots, t_m] \\ g^{(m)}[F(t_1), \cdots, F(t_m)], t = \{t_1, \cdots, t_m\}, \end{cases} \tag{12}$$

and the elementary integral can be written as

$$\theta_s(\tau) = J_{0,s}, \theta_s(\sigma) = J_{i,s},$$
$$\theta_s(t) = \begin{cases} \int_0^s du(\prod_{j=1}^m \theta_u(t_j)), t = [t_1, \cdots, t_m] \\ \int_0^s \circ dW_i(u)(\prod_{j=1}^m \theta_u(t_j)), t = \{t_1, \cdots, t_m\}. \end{cases} \tag{13}$$

Fig.1(a) illustrates the elementary weight, derivative and integral graphically.

$t = [\sigma, [\{\sigma\}, [\tau, \sigma]]]$

$a(t) = 2^3 \times (\frac{1}{0!})^3(\frac{1}{1!})^2(\frac{1}{2!})^3 = 1$

$F(t) = f''(g, f''(g'g, f''(f, g)))$

$\quad = f^i_{jk}g^j f^k_{lm}g^l_n g^n f^m_{np} f^n g^p$

$\theta_h(t) = \int_0^h ds_1 J_{j,s_1} \int_0^{s_1} ds_2 J_{nl,s_2} \int_0^{s_2} ds_3 J_{0,s_3} J_{p,s_3}$

(a)

$\delta x_i(h) = \bullet + \circ + \Big| + \Big| + \Big| + \Big|$

$+ \cdots$

(b)

Figure 1: Illustration of the BRT method. Fig.1(a) shows a bicolour rooted tree t, and its elementary weight $a(t)$, derivative $F(t)$ and integral $\theta_h(t)$, respectively. Fig.1(b) shows the 0th and 1st derivative terms of stochastic Taylor expansion of $\delta x_i(h)$ by the BRT method.

Therefore the stochastic Taylor expansion is given by

$$\delta x_i(h) = \sum_{t \in T} a(t)F(t)\theta_h(t)$$
$$= sum\ of\ all\ the\ non\text{-}isomorphic$$
$$bicolour\ rooted\ trees, \tag{14}$$

where T is the set of non-isomorphic bicolour rooted trees. Fig.1(b) illustrates how to use this formula to express $\delta x_i(h) = \delta x_i^0(h) + \delta x_i^1(h) + \cdots$.

3. Algorithm

Due to the complexity of stochastic Taylor expansion, we only consider Langevin equation (LE) which plays an important part in the fields involving randomness in this paper. An N dimensional set of coupled LEs has the form

$$\ddot{q}_i = -\frac{\partial V(\mathbf{q}(t))}{\partial q_i} - \gamma_i \dot{q}_i + \xi_i(t), \tag{15}$$

where $V(\mathbf{q}(t))$ is the external potential, $\gamma_i(i = 1, \cdots, N)$ is a set of friction parameters, $\xi_i(t)$ is random noise with zero mean, the correlation relation is

$$< \xi_i(t)\xi_j(t') > = 2\gamma_i T \delta_{ij}\delta(t - t'), \tag{16}$$

and the Hamilton canonical equations are

$$\dot{q}_i = p_i,$$
$$\dot{p}_i = -\frac{\partial V(\mathbf{q}(t))}{\partial q_i} - \gamma_i p_i + \xi_i(t). \tag{17}$$

The form of Eq.(17) where only every second equation has a noise term with constant diffusion coefficient, as well as the potential $V(\mathbf{q}(t))$ is unrelated to $\mathbf{p}(t)$, makes it possible to sharply decrease the complexity of Eq.(14) so as to obtain a high order algorithm for LE.

For the Eq.(17), we can translate it into the form

$$\dot{x}_i = f_i(X(t)) + g_i\xi_i(t) \quad (i = 1, 2, ..., 2N)$$
$$< \xi_i(t)\xi_j(t') > = \delta_{ij}\delta(t - t'), \tag{18}$$

where $f_i(X(t))$ is equal to x_{i+1} for odd i and to $-\partial V(\mathbf{X}(t))/\partial x_{i-1} - \gamma_i x_i$ for even i, $\mathbf{X}(t) = \{x_1, x_3, ..., x_{2N-1}\}$, g_i is a set of constants with $g_i = 0$

if i is odd number. Because of the property of $V(\mathbf{q}(t))$, one can find that $f^i_{jk} \neq 0$ only if j and k are both odd numbers. From above properties, a key property for the simplification of the stochastic Taylor expansion, that is, $\cdots f^i_{jk} g_j \cdots = 0$, can be found. We can rewrite it in the compact form as follow:

$$\cdots, [\cdots, \sigma, \cdots], \cdots = 0, \tag{19}$$

so if a bicolour rooted tree has this structure, it should have no contribution to the stochastic Taylor expansion.

From the analysis above, one can obtain a general method for solving the Langevin equation numerically. If we want to get a numerical method to the order $o(m,n)$, we should:

(a)For the deterministic part:

Solve it by the standard Runge-Kutta method of order m.

(b)For the stochastic part:

(i)Write down all the non-isomorphic bicolour rooted trees that can avoid the structure (19);

(ii)Attach each vertex with white or black so as to make the tree have order n.

(c)Add up the results of (a) and (b).

Using these three criteria, all the terms up to order $o(7,4.5)$ are,

$$\begin{aligned}
\delta x_{idet}(h) =& \sum_{j=0}^{6} RK(j), \\
\delta x_{iran}(h) =& \sigma + [\sigma] + [[\sigma]] + [[[\sigma]]] + [\tau, [\sigma]] \\
& + [[[[\sigma]]]] + [\tau, [[\sigma]]] + [[\tau], [\sigma]] \\
& + [\tau, \tau, [\sigma]] + [[\tau, [\sigma]]] + [[\sigma], [\sigma]], \\
\delta x_i(h) =& \delta x_{idet}(h) + \delta x_{iran}(h).
\end{aligned} \tag{20}$$

where the $RK(j), (j = 0, \cdots, 6)$ are the BRTs with $j+1$ deterministic nodes only which are identical to the terms of standard Runge-Kutta method for ODEs. These terms compose the deterministic part of our algorithm, and we can use Runge-Kutta method to solve the deterministic part numerically [17, 19].

Then we try to find a way to calculate the stochastic part in Eq.(20). We here introduce a method to approximate the elementary integral which is developed by P. E. Kloeden and E. Platen [18]. They showed that if

$\mathbf{W}(t) = (W_1(t), \cdots, W_N(t))$ is an N-dimensional Wiener process on the time interval $[0, h]$, the componentwise Fourier expansion of the Brownian bridge process $\mathbf{W}(t) - \frac{t}{h}\mathbf{W}(h)$ is

$$W_i(t) - \frac{t}{h}W_i(h) = \frac{1}{2}a_{i0} + \sum_{j=1}^{\infty}(a_{ij}\cos(\frac{2j\pi t}{h}) + b_{ij}\sin(\frac{2j\pi t}{h})), \qquad (21)$$

where a_{ij}, b_{ij} are $N(0, h/2\pi^2 j^2)$ distributed and pairwise independent, then setting $t = 0$ in the equation (21) gives $a_{i0} = -2\sum_{j=1}^{\infty} a_{ij} \equiv a_i^0$.

Now, we begin to calculate the stochastic part of Eq.(20). Firstly, let us set the $\mathbf{W}(0) = 0$, then use equation (21), we can easily find that

$$\sigma = a(\sigma)F(\sigma)\theta_h(\sigma) = g^i J_{i,h} = g^i W_i(h) \equiv g^i \omega_i^1,$$

$$[\sigma] = f_j^i g^j J_{j0,h} = f_j^i g^j \int_0^h ds_1 \int_0^{s_1} \circ dW_j(s_2)$$

$$= f_j^i g^j \int_0^h W_j(s_1) ds_1 \qquad (22)$$

$$= h f_j^i g^j (\frac{W_j(h)}{2} + \frac{a_j^0}{2})$$

$$\equiv h f_j^i g^j \omega_j^2,$$

where $W_i(h) \equiv W_i$ is a set of independent Gaussian random variables sampled from $N(0, h)$. Similarly calculation gives

$$[[\sigma]] = h^2 f_j^i f_k^j g^k \omega_k^3$$

$$[[[\sigma]]] = h^3 f_j^i f_k^j f_l^k g^l \omega_l^4$$

$$[\tau, [\sigma]] = h^3 f_{jk}^i f^j f_l^k g^l \omega_l^5$$

$$[[[[\sigma]]]] = h^4 f_j^i f_k^j f_l^k f_m^l g^m \omega_m^6$$

$$[\tau, [[\sigma]]] = h^4 f_{jk}^i f^j f_l^k f_m^l g^m \omega_m^7$$

$$[[\tau], [\sigma]] = h^4 f_{jk}^i f_l^j f^l f_m^k g^m \omega_m^8 \qquad (23)$$

$$[\tau, \tau, [\sigma]] = \frac{h^4}{2} f_{jkl}^i f^j f^k f_m^l g^m \omega_m^9$$

$$[[\tau, [\sigma]]] = h^4 f_j^i f_{kl}^j f^k f_m^l g^m \omega_m^{10}$$

$$[[\sigma], [\sigma]] = \frac{h^3}{2} f_{jk}^i f_l^j g^l f_m^k g^m \Omega_{lm}^1$$

9

where

$$\omega_i^3 = \frac{W_i}{6} + \frac{a_i^0}{4} + \frac{b_i^1}{2}$$

$$\omega_i^4 = \frac{W_i}{24} + \frac{a_i^0}{12} + \frac{a_i^1}{4} + \frac{b_i^1}{4}$$

$$\omega_i^5 = \frac{W_i}{8} + \frac{a_i^0}{6} - \frac{a_i^1}{4} + \frac{b_i^1}{4}$$

$$\omega_i^6 = \frac{W_i}{120} + \frac{a_i^0}{48} + \frac{a_i^1}{8} + \frac{b_i^1}{12} - \frac{b_i^2}{8}$$

$$\omega_i^7 = \frac{W_i}{30} + \frac{a_i^0}{16} + \frac{a_i^1}{8} + \frac{b_i^1}{6} + \frac{b_i^2}{8}$$

$$\omega_i^8 = \frac{W_i}{20} + \frac{a_i^0}{16} - \frac{a_i^1}{8} + \frac{b_i^1}{12} - \frac{b_i^2}{8} \tag{24}$$

$$\omega_i^9 = \frac{W_i}{10} + \frac{a_i^0}{8} - \frac{a_i^1}{4} + \frac{b_i^1}{6} - \frac{b_i^2}{4}$$

$$\omega_i^{10} = \frac{W_i}{40} + \frac{a_i^0}{24} + \frac{b_i^1}{12} + \frac{b_i^2}{4}$$

$$a_i^0 = -2 \sum_{j=1}^{\infty} a_{ij}, \; b_i^1 = \sum_{j=1}^{\infty} \frac{1}{\pi j} b_{ij},$$

$$a_i^1 = \sum_{j=1}^{\infty} \frac{1}{(\pi j)^2} a_{ij}, \; b_i^2 = \sum_{j=1}^{\infty} \frac{1}{(\pi j)^3} b_{ij},$$

and the first non-Gaussian random variable is

$$\Omega_{ij}^1 = \omega_i^1 \omega_j^9 + a_i^0 \omega_j^5 - \frac{\omega_i^1 \omega_j^1}{20} - \frac{a_i^0 a_j^0}{12} - \frac{a_i^0 \omega_j^1}{8} + \frac{b_i^1 b_j^1}{4} + \frac{c_{ij}}{8},$$

$$c_{ij} = \sum_{k=1}^{\infty} \frac{1}{(\pi k)^2} (a_{ik} a_{jk} + b_{ik} b_{jk}). \tag{25}$$

We can find that there are only 5 independent variables among $\omega_i^j, (j = $

$1, \cdots, 10$). Let's choose $\omega_i^1, \omega_i^2, \omega_i^3, \omega_i^4, \omega_i^6$ as the independent variables, then

$$\omega_i^5 = \omega_i^3 - \omega_i^4$$
$$\omega_i^7 = \omega_i^4 - \omega_i^6$$
$$\omega_i^8 = \frac{1}{2}\omega_i^3 - \omega_i^4 + \omega_i^6 \qquad (26)$$
$$\omega_i^9 = \omega_i^3 - 2\omega_i^4 + 2\omega_i^6$$
$$\omega_i^{10} = \omega_i^4 - 2\omega_i^6$$

Now, the last procedure we should do is to determine the five Gaussian random variables $W_i, a_i^0, a_i^1, b_i^1, b_i^2$ and the non-Gaussian random variable c_{ij}. We truncate c_{ij} to the first term, that is, $c_{ij} \approx (a_{i1}a_{j1} + b_{i1}b_{j1})/\pi^2$. Since W_i, a_{ij}, b_{ij} are independent and $W_i \sim N(0, h)$, $a_{ij} \sim N(0, h/2\pi^2 j^2)$, $b_{ij} \sim N(0, h/2\pi^2 j^2)$, we can see that

$$a_i^0 \sim N(0, \frac{h}{3}), \ b_i^1 \sim N(0, \frac{h}{180}),$$
$$a_i^1 \sim N(0, \frac{h}{1890}), \ b_i^2 \sim N(0, \frac{h}{18900}),$$
$$< a_i^0 a_i^1 >= -\frac{h}{90}, \ < a_i^0 a_{i1} >= -\frac{h}{\pi^2}, \ < a_i^1 a_{i1} >= \frac{h}{2\pi^4}, \qquad (27)$$
$$< b_i^1 b_i^2 >= \frac{h}{1890}, \ < b_i^1 b_{i1} >= \frac{h}{2\pi^3}, \ < b_i^2 b_{i1} >= \frac{h}{2\pi^5}.$$

Let $\phi_i^1, \phi_i^2, \phi_i^3, \phi_i^4, \phi_i^5, \phi_i^6, \phi_i^7$ to be seven independent standard Gaussian random variables, then use Eq.(27), we can get

$$W_i = \sqrt{h}\phi_i^1$$
$$a_i^0 = \sqrt{\frac{h}{3}}\phi_i^2$$
$$a_i^1 = \frac{\sqrt{h}}{30}(-\frac{\phi_i^2}{\sqrt{3}} + \frac{\phi_i^3}{\sqrt{7}})$$
$$b_i^1 = \sqrt{\frac{h}{180}}\phi_i^4 \qquad (28)$$
$$b_i^2 = \frac{\sqrt{h}}{63}(\frac{\phi_i^4}{\sqrt{5}} + \frac{\phi_i^5}{10})$$
$$a_{i1} = \sqrt{h}(-0.175493\phi_i^2 + 0.139348\phi_i^3 + 0.0210906\phi_i^6)$$
$$b_{i1} = \sqrt{h}(0.21635\phi_i^4 + 0.0617995\phi_i^5 + 0.00584342\phi_i^7)$$

11

The BRT method gives an algorithm for the Langevin equation so long as we determine the deterministic and the stochastic part of Eq.(20) respectively and add up each other. The deterministic part can be solved by the standard Runge-Kutta algorithm [19], and the stochastic part can be solved by the Eqs.(22)-(23).

4. Numerical simulations

4.1. Energy relaxation in double well

To verify the validity of our algorithm, the Kramers equation will be considered as the severe test for our algorithm. The form is as follow:

$$
\begin{aligned}
\dot{q}(t) &= p(t), \\
\dot{p}(t) &= -V^{'}(q(t)) - \gamma p(t) + \xi(t),
\end{aligned}
\tag{29}
$$

and $\xi(t)$ is the Gaussian random force obeying the fluctuation dissipation theorem

$$
< \xi(t)\xi(t^{'}) >= 2\gamma T.
\tag{30}
$$

Our method implies that the algorithm for Eqs.(29)-(30) is,

$$
\begin{aligned}
q(t+h) &= q_{det}(q(t), p(t), h) + q_{ran}(q(t), p(t), h), \\
p(t+h) &= p_{det}(q(t), p(t), h) + p_{ran}(q(t), p(t), h),
\end{aligned}
\tag{31}
$$

where $q_{det}(q(t), p(t), h)$ and $p_{det}(q(t), p(t), h)$ are the results of evolving the equations in the period 0-h by the seventh-order Runge-Kutta algorithm [19] which is used in the ODE, and the stochastic part of Eq.(31) is,

$$
\begin{aligned}
q_{ran}(q(t), p(t), h) =& \sqrt{2\gamma T}[(h\omega_2^2 - h^2\gamma\omega_2^3 + h^3\gamma^2\omega_2^4 - h^4\gamma^3\omega_2^6) \\
&+ (-h^3\omega_2^4 + 2h^4\gamma\omega_2^6)V^{''} - h^4 p(t)\omega_2^{10}V^{'''}], \\
p_{ran}(q(t), p(t), h) =& \sqrt{2\gamma T}[(\omega_2^1 - h\gamma\omega_2^2 + h^2\gamma^2\omega_2^3 - h^3\gamma^3\omega_2^4 \\
&+ h^4\gamma^4\omega_2^6) + (-h^2\omega_2^3 + 2h^3\gamma\omega_2^4 - 3h^4\gamma^2\omega_2^6)V^{''} \\
&+ (-h^3 p(t)\omega_2^5 + h^4\gamma p(t)\omega_2^7 + h^4\gamma p(t)\omega_2^8 \\
&+ h^4\gamma p(t)\omega_2^{10})V^{'''} + h^4 V^{''}V^{''}\omega_2^6 + h^4 V^{'}V^{'''}\omega_2^8 \\
&- \frac{h^4}{2}V^{''''}p^2(t)\omega_2^9] - h^3\gamma T V^{'''}\Omega_{22}^1,
\end{aligned}
\tag{32}
$$

where $\omega_2^i(i = 1, \cdots, 10)$ and Ω_{22}^1 have been defined in the previous section.

The double well potential in this example is,

$$V(q) = q^4 - 2q^2. \tag{33}$$

It has two minima located at $q = \pm 1$ and a potential barrier with the height $\Delta V = 1$ between the two wells. The friction coefficient γ is set to 1. The initial condition is chosen on the top of the barrier. The average is taken over 5000 realizations of the Gaussian random force during the trajectory. Fig.2 shows the result which is compared with the Euler method and the Heun method [20]. We perform these three methods at T=0.05 and T=0.2 respectively. We find that the results of these three different methods are almost agreed. Nevertheless, the step size of our method, Heun method and Euler method are 0.1, 0.001 and 0.0001, respectively. The Kramers equation has been simulated extensively by many authors (Ref. [15] and the references therein). As for the convergence, we compare our algorithm with previous algorithms here. Fig.(3) shows the convergence of the three algorithms for solving the Kramers equation. It is evident that our algorithm diverges slowly than the other algorithms as the step size increases.

4.2. Stochastic resonance

Stochastic resonance, which is originally developed to explain the ice ages [21, 22], has spread well beyond physics and left its fingerprints in many other research areas [23, 24], such as complex networks [25], biological systems [26], neuroscience [27, 28] and quantum computing [29]. The governing equations in these very different fields are essentially Langevin equation or its generalizations. We present an example of stochastic resonance in neuroscience to demonstrate our algorithm in the case of time-dependent Langevin equation with the Ornstein-Uhlenbeck noise [23]. An enlightening model in the neuronal dynamical systems is the noise-driven bistable system whose equations can be described as follow:

$$\begin{aligned} &\ddot{x} + \gamma\dot{x} = -V^{'}(x) + A\cos(\omega t) + \varepsilon(t), \\ &< \varepsilon(t)\varepsilon(t^{'}) >= D\lambda\exp(-\lambda|t - t^{'}|), \end{aligned} \tag{34}$$

where $\varepsilon(t)$ is the Ornstein-Uhlenbeck noise with intensity D and the inverse of characteristic time λ, and the system is driven by an external periodic force with amplitude A and frequency ω.
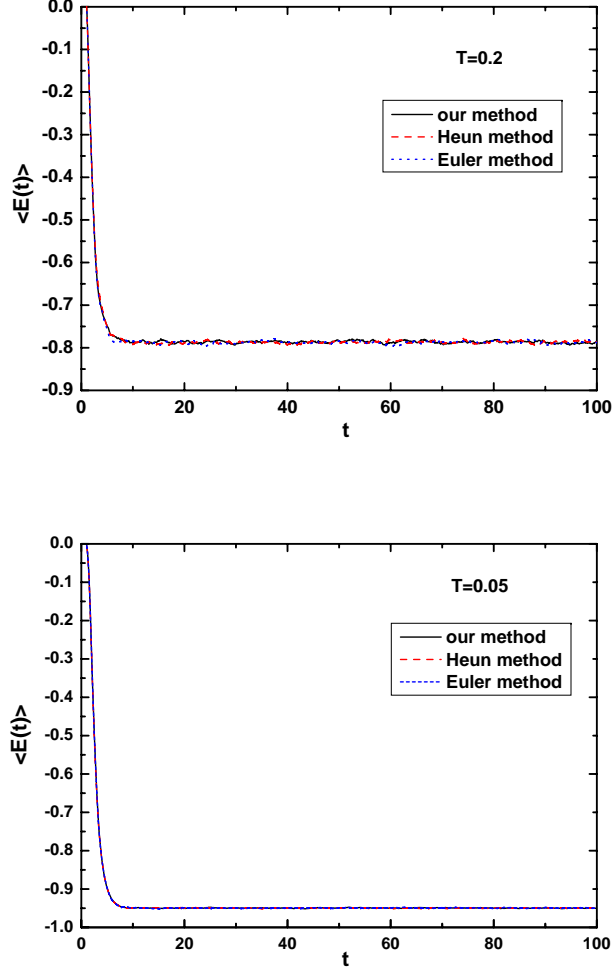
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Figure 2: Comparison of different numerical methods for solving the energy relaxation in the double well potential. The friction coefficient γ is equal to 1. The average is taken over 5000 realizations for all the algorithms. The solid line is our method with step size 0.1, the dash line is the Heun method with step size 0.001, and the short dash line is the Euler method with the step size 0.0001. Panel a shows the relaxation at high temperature T=0.2 and panel b shows the relaxation at low temperature T=0.05, respectively.
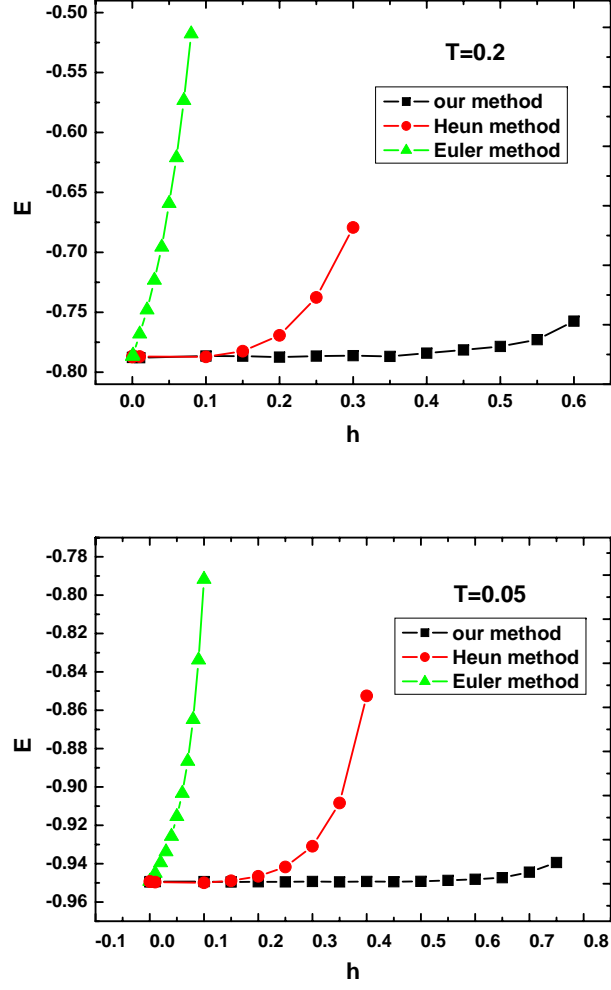
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Figure 3: The convergence of different numerical methods for solving the Kramers equation. The friction coefficient γ is equal to 1. E is the average energy at a certain temperature and h is the step size. Panel a shows the convergence at high temperature T=0.2 and panel b shows the convergence at low temperature T=0.05, respectively.

To use our algorithm to solve Eq.(34) numerically, we should first transform it into,

$$\begin{aligned}
\dot{y} &= 1, \\
\dot{x} &= p, \\
\dot{p} &= -\gamma p - V^{'}(x) + A\cos(\omega y) + \varepsilon, \\
\dot{\varepsilon} &= -\lambda\varepsilon + \lambda\sqrt{2D}\xi(t), \\
&< \xi(t)\xi(t^{'}) >= \delta(t - t^{'}).
\end{aligned} \tag{35}$$

Let $y \rightarrow x_1, x \rightarrow x_2, p \rightarrow x_3, \varepsilon \rightarrow x_4$, we can further simplify Eq.(35) into a compact form,

$$\begin{aligned}
\dot{x}_i &= f_i(X(t)) + g_i\xi_i(t) \quad (i = 1, 2, 3, 4), \\
&< \xi(t)\xi(t^{'}) >= \delta(t - t^{'}),
\end{aligned} \tag{36}$$

with

$$\begin{aligned}
&f_1(X(t)) = 1, f_2(X(t)) = x_3, f_4(X(t)) = -\lambda x_4, \\
&f_3(X(t)) = -\gamma x_3 - V^{'}(x_2) + A\cos(\omega x_1) + x_4, \\
&g_1 = g_2 = g_3 = 0, \; g_4 = \lambda\sqrt{2D},
\end{aligned} \tag{37}$$

then one can easily find that property (19) is held again.

Accordingly, the numerical method of Eqs.(36)-(37) can be written as follow:

$$\begin{aligned}
x_1(t + h) &= x_{1det}(X(t), h) + x_{1ran}(X(t), h), \\
x_2(t + h) &= x_{2det}(X(t), h) + x_{2ran}(X(t), h), \\
x_3(t + h) &= x_{3det}(X(t), h) + x_{3ran}(X(t), h), \\
x_4(t + h) &= x_{4det}(X(t), h) + x_{4ran}(X(t), h),
\end{aligned} \tag{38}$$

where the deterministic part of Eq.(38) accords with the Ronge-Kutta algo-

rithm for the ODEs, and the stochastic part of Eq.(38) is

$$
\begin{aligned}
x_{1ran}(X(t), h) &= 0, \\
x_{2ran}(X(t), h) &= \lambda\sqrt{2D}[(h^2\omega_4^3 - h^3(\gamma + \lambda)\omega_4^4 \\
&\quad + h^4(\gamma^2 + \gamma\lambda + \lambda^2)\omega_4^6) - h^4\omega_4^6 V''], \\
x_{3ran}(X(t), h) &= \lambda\sqrt{2D}[(h\omega_4^2 - h^2(\gamma + \lambda)\omega_4^3 \\
&\quad + h^3(\gamma^2 + \gamma\lambda + \lambda^2)\omega_4^4 - h^4(\gamma^3 + \gamma^2\lambda \\
&\quad + \gamma\lambda^2 + \lambda^3)\omega_4^6) + (-h^3\omega_4^4 + h^4(2\gamma + \lambda)\omega_4^6)V'' \\
&\quad - h^4 x_3(t)\omega_4^7 V'''], \\
x_{4ran}(X(t), h) &= \lambda\sqrt{2D}[\omega_4^1 - h\lambda\omega_4^2 + h^2\lambda^2\omega_4^3 \\
&\quad - h^3\lambda^3\omega_4^4 + h^4\lambda^4\omega_4^6].
\end{aligned}
\tag{39}
$$

The double well potential in this example is,

$$
V(x) = -\frac{1}{2}x^2 + \frac{1}{4}x^4,
\tag{40}
$$

and the periodic driven force's amplitude A and frequency ω are 0.03 and 0.01 respectively. We consider the relation between the amplitude of output of the system $< x >$ and the noise intensity D. The average is taken over 5×10^5 realizations and the Heun method is used as a comparison. We then compare our results with the model mentioned in [23]:

$$
\begin{aligned}
\dot{x} &= -V'(x) + A\cos(\omega t) + \xi(t), \\
< \xi(t)\xi(t') > &= 2D\delta(t - t').
\end{aligned}
\tag{41}
$$

The theoretical result of $< x >$ in this model is $< x >= \frac{A}{D}\frac{2r_k}{\sqrt{4r_k^2 + \omega^2}}$, where $r_k = \frac{1}{\sqrt{2\pi}}\exp\left(-\frac{\Delta V}{D}\right)$.

Fig.(4) shows the results of our simulations. The black line and the red line are the simulations of our method with step size 0.1 and the Heun method with step size 0.01 respectively, with the parameters γ and λ equal to 1. We now see that the results of our method and the Heun method are almost the same, however, the step size of our method is larger than the one used in Heun method. The parameters of the green line is the same as the black line except $\lambda = 10$, that is, the characteristic time is shorter, and in this condition, the Ornstein-Uhlenbeck noise is closer to the Gaussian noise. We
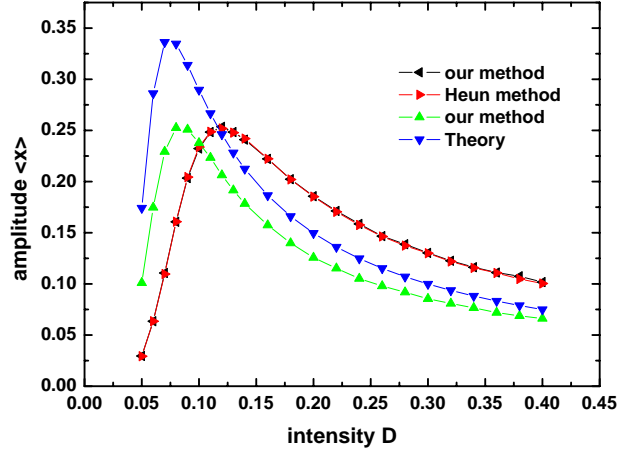
17

Figure 4: Comparison of different numerical methods for the stochastic resonance in the noise-driven bistable system. The periodic driven force's amplitude A and frequency ω are 0.03 and 0.01, respectively. The friction coefficient γ is equal to 1. The amplitude of output is averaged over 5×10^5 trajectories. The black line is our method with step size 0.1 and the red line is the Heun method with step size 0.01. Both the two lines have the characteristic time 1. The green line is our method with step size 0.1 and characteristic time 0.1. The blue line is the theoretical result of Eq.(41).

can find that the *resonant noisy intensity* (the maximum of the line) shifts left when we shorten the characteristic time. In other words, lengthening the characteristic time can enhance the noise resistance of the system. The blue line is the theoretical result of Eq.(41). Since the influence of the inertia term $\ddot{x}$, we can see that the amplitude of output $< x >$ of the theoretical result is greater than our numerical result as shown in the green line.

5. Conclusion

We have proposed the bicolour rooted tree method to do the stochastic Taylor expansion systematically. This method can be used to solve the stochastic differential equation numerically. In this paper, we focus on the Langevin equation which is widely used in modern science. A high order algorithm $o(7,4.5)$ is derived in this paper. Comparing with other usual algorithms, our method is advantageous in computational efficiency and accuracy. We present our method in the two examples. In the first example of energy relaxation in the double well, we show our method gives the same results as presented in other papers, and the convergence is better than the other algorithms. In the second example, we propose an algorithm for the time-dependent Langevin equation with the Ornstein-Uhlenbeck noise, and the result of our algorithm is the same as the one obtained by Heun method. It shows our algorithm is suitable for the Langevin equation regardless of the time-dependence of the equation. However, the readers should note that we only provide the algorithm for Eq.(17) which satisfies the property (19) since this property can drastically reduce the complexity of Eq.(14). For the other type of SDEs that the property (19) can not be held, such as the Hodgkin-Huxley model in neuroscience [27], interested readers can design their own algorithms based on the Eq.(14). For the purpose of using our method in the more difficult situations, one can consider the case that the diffusion coefficients are variable. All in all, we have provided a systematic scheme for searching the high order algorithm for the SDE and find that it can reduce drastically when deal with the Langevin equation.

Acknowledgments

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